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4. TITLE AND SUBTITLE Massively Parallel Complete Active Space Self Consistent Field Molecular Dynamics		5. FUNDING NUMBERS N00014-93-1-0908		
6. AUTHOR(S) Emily A. Carter				
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Department of Chemistry and Biochemistry Univ of California, Los Angeles 405 Hilgard Avenue Los Angeles, CA 90024-1406		8. PERFORMING ORGANIZATION REPORT NUMBER		
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13. ABSTRACT (Maximum 200 words) This report briefly summarizes the research developments in ab initio dynamics made possible by this augmentation award to the parent ONR grant. A full description of the research accomplishments will appear in the final technical report of the parent grant (due 14 March 1998).				
14. SUBJECT TERMS Ab initio dynamics; pseudospectral; local correlation.		15. NUMBER OF PAGES 2		
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FINAL TECHNICAL REPORT

and

ANNUAL AASERT REPORT (FORM A2-2)

TO THE OFFICE OF NAVAL RESEARCH

For Grant No. N00014-93-1-0908

Emily A. Carter

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Los Angeles, CA 90095-1569

Summary

This AASERT grant supported, off and on, six graduate students and one undergraduate student. These were, of course, all U.S. citizens, including 3 women and 1 Asian-American. The work done by these students led to publications on complete active space self-consistent field molecular dynamics simulations on clusters and chemical reactions, local pseudospectral electron correlation methods, and developments in pseudospectral electronic structure theory. The latter include a systematic means of eliminating aliasing errors in conventional pseudospectral self-consistent field theory and a new massively parallel pseudospectral self-consistent field scheme that also eliminates the aliasing problem while still reducing the scaling of the self-consistent field algorithm by solving an unconventional minimization problem. These accomplishments will be summarized in detail in the final technical report of the parent grant.

FORM A2-2

**AUGMENTATION AWARDS FOR SCIENCE & ENGINEERING RESEARCH TRAINING (AASERT)
REPORTING FORM**

The Department of Defense (DOD) requires certain information to evaluate the effectiveness of the AASERT program. By accepting this Grant Modification, which bestows the AASERT funds, the Grantee agrees to provide the information requested below to the Government's technical point of contact by each annual anniversary of the AASERT award date.

1. Grantee identification data: (R & T and Grant numbers found on Page 1 of Grant)

- a. University of California, Los Angeles
University Name
- b. N00014-93-1-0908 c. 412W005---02
Grant Number R & T Number
- d. Emily A. Carter e. From: 6/1/96 To: 5/31/97
P.I. Name AASERT Reporting Period

NOTE: Grant to which AASERT award is attached is referred to hereafter as "Parent Agreement."

2. Total funding of the Parent Agreement and the number of full-time equivalent graduate students (FTEGS) supported by the Parent Agreement during the 12-month period prior to the AASERT award date.

- a. Funding: \$84,615
- b. Number FTEGS: 0.75

3. Total funding of the Parent Agreement and the number of FTEGS supported by the Parent Agreement during the current 12-month reporting period.

- a. Funding: \$76,152
- b. Number FTEGS: 0.75

4. Total AASERT funding and the number of FTEGS and undergraduate students (UGS) supported by AASERT funds during the current 12-month reporting period.

- a. Funding: \$65,000
- b. Number FTEGS: 3
- c. Number UGS: 0

VERIFICATION STATEMENT: I hereby verify that all students supported by the AASERT award are U.S. citizens.

Emily A. Carter
Principal Investigator

Sept. 10, 1997
Date